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Final Report: SHORT-TERM INNOVATIVE RESEARCH (STIR) PROGRAM:"Synthesizing new functional 2D semiconducting solids"

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14. ABSTRACT

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RPPR Final Report
as of 17-Sep-2018

Agency Code:

Proposal Number: 69060MSII **Agreement Number: W911NF-16-1-0186**
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Final Report for Period Beginning 01-May-2016 and Ending 31-Jan-2017
Title: SHORT-TERM INNOVATIVE RESEARCH (STIR) PROGRAM:"Synthesizing new functional 2D semiconducting solids"
Begin Performance Period: 01-May-2016 **End Performance Period:** 31-Jan-2017
Report Term: 0-Other
Submitted By: Madhusudan Menon Email: super250@uky.edu
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Distribution Statement: 1-Approved for public release; distribution is unlimited.

STEM Degrees: 2 **STEM Participants:** 0

Major Goals: Experimental synthesis of a new class of 2D material that is one atom thick and flat following the theoretical guidance as part of the exploratory research.

Accomplishments: We attempted the growth of 2D SiC on polycrystalline copper rolls using our Chemical Vapor Deposition (CVD) reactor. During the growth process, both CH4 and SiH4 gases were introduced. The specific objective was to create a stable isolated single layer of the SiC material. The Raman spectrum of the sample grown on copper roll at 1000 C with combined flows of CH4 and SiH4 were analzsed. The TEM images confirmed the presence of both C and Si. Most interestingly, Raman spectrum showed SiC like features in the peaks. These results are significant and confirm growth of at least regions of 2D SiC structures.

Training Opportunities: Graduate students were involved in the experimental effort performing Raman studies.

Results Dissemination: Nothing to Report

Honors and Awards: Nothing to Report

Protocol Activity Status:

Technology Transfer: Nothing to Report

PARTICIPANTS:

Participant Type: Faculty
Participant: Mahendra Sunkara Prof
Person Months Worked: 1.00 **Funding Support:**
Project Contribution:
International Collaboration:
International Travel:
National Academy Member: N
Other Collaborators:

RPPR Final Report
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Participant Type: Graduate Student (research assistant)
Participant: Rong Zhao
Person Months Worked: 6.00 **Funding Support:**
Project Contribution:
International Collaboration:
International Travel:
National Academy Member: N
Other Collaborators:

Participant Type: Graduate Student (research assistant)
Participant: Daniel Jaramillo
Person Months Worked: 6.00 **Funding Support:**
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Other Collaborators:

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Date Submitted: Date Published:
Publication Location:
Article Title: Structural, electronic and mechanical properties of Si2BN under uniaxial strain: an ab-initio study'
Authors: Z. G. Fthenakis and M. Menon
Keywords: nanomechanics, molecular dynamics, first principles calculations
Abstract: Si2BN has been recently predicted theoretically as a new entirely planar 2-dimensional metallic material which is stable even at T> 1000 K. It was also found that it is metallic, with few states at the Fermi level and similar electronic properties at the Fermi level as silicene. In the present work we study its structural, electronic and mechanical properties under tensile strain till the fracture limit and compare them to the corresponding properties for graphene. According to our findings, the metallic character of Si2BN is enhanced as a function of strain, since strain introduces several conduction states into the valence band. Study of its mechanical properties reveals Si2BN to be anisotropic, while exhibiting large values of Young's modulus. Furthermore, structurally it is found to be very robust and comparable to graphene.
Distribution Statement: 1-Approved for public release; distribution is unlimited.
Acknowledged Federal Support: **Y**

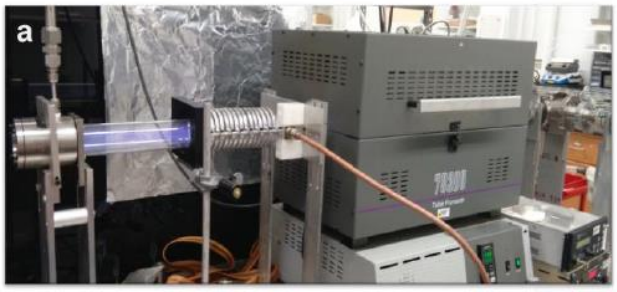

FIGURE 1. CVD system used for growth of 2D SiC

We have attempted growth of 2D SiC on polycrystalline copper foils using our Chemical Vapor Deposition (CVD) reactor as shown in Fig. 1. During the growth process, both CH_4 and SiH_4 gasses were introduced after annealing the copper substrate in a H_2/Ar flow at 1000 ^{0}C. However, due to safety reasons and to facilitate slow growth rate, we have used very dilute SiH_4 (2 mol. %) in hydrogen. This imposed the restriction of using low concentrations of methane. Our preliminary results showed formation of graphene at ultra-low concentration of methane (<0.5 sccm compared to 20 sccm typically used for graphene synthesis). Since carbon solubility in copper is extremely low compared to that of Si, we maintained SiH_4 throughout the cooling process even after the CH_4 flow was turned off. Fig. 2 shows (a) low magnification TEM image (b) high magnification TEM image (c) EDX spectrum (d) Raman spectrum of the sample grown on copper foil at 1000 ^{0}C with combined flows of CH_4 and SiH_4. TEM images confirm the presence of layered structure while EDX confirms presence of both C and Si. Most interestingly, Raman spectrum shows SiC like feature (~860 cm^{-1}) in addition to typical D, G, and 2D peaks characteristic to graphene. These initial results are encouraging and confirms growth of at least regions of 2D SiC structures. We are planning to perform more in-depth characterization of the material and to reproduce the results.

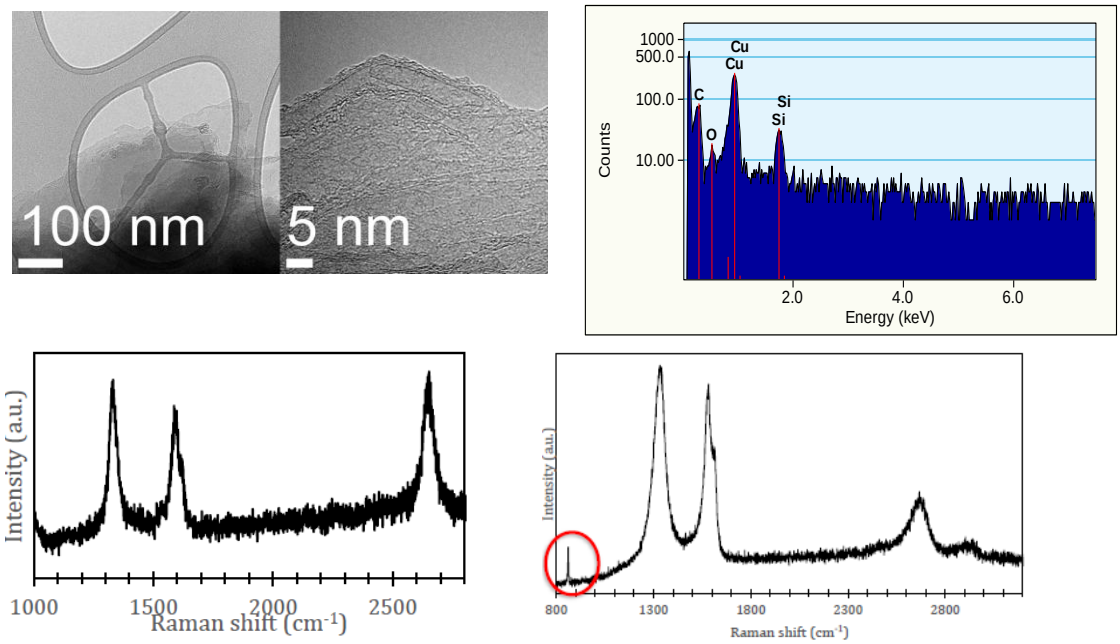

FIGURE 2. Characterization results from preliminary 2D SiC synthesis experiments: (a) low magnification TEM image (b) high magnification TEM image (c) EDX spectrum (d) Raman spectra for samples with and without SiH_4 showing SiC like peak in addition to graphene peaks when SiH4 is present.

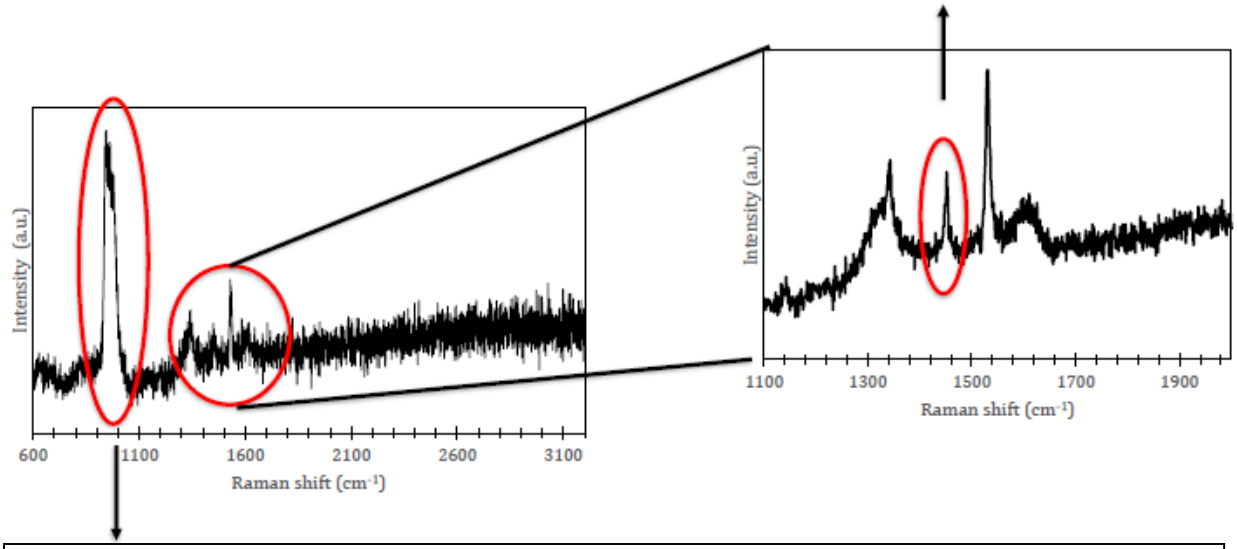

FIGURE 3. Raman spectrum for a samples synthesized with CH_4 and SiH_4 showing additional peak between the D and G peaks of graphene.

Under varying conditions for CH_4 and SiH_4 residency times during the reduction, growth, and cooling processes we synthesized 2D materials which shows an additional Raman peak between D and G bands of graphene as shown in Fig. 3. Currently we are trying to understand the origin of this peak with additional characterizations.